

The TBA, the Gross-Neveu Model, and Polyacetylene

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Abstract. We summarize recent work showing how the Thermodynamic Bethe Ansatz may be used to study the finite-density first-order phase transition in the Gross-Neveu model. The application to trans-polyacetylene is discussed, and the significance of the results is addressed.

In this contribution, rather than simply repeat what is contained in the literature, we should like to attempt to place this work in context, and to emphasize those points that are either the most novel or the most inviting of further investigation. Details of calculation can be found in the published references (Chodos and Minakata 1994, 1997).

This work brings together three disparate elements: the Gross-Neveu (GN) model, the thermodynamic Bethe Ansatz (TBA), and the phenomenology of polyacetylene $((CH)_x)$.

Polyacetylene is essentially a linear chain which comes in two forms, dubbed *trans* and *cis*. The *trans* form, which is the more stable, has a doubly-degenerate ground state. It is this circumstance that allows for the existence of topological excitations, or solitons, and these lead in turn to a rich phenomenology. An excellent review of polyacetylene and other similar polymers is the article in Reviews of Modern Physics by Heeger, Kivelson, Schrieffer and Su (1988).

It was realized long ago, by Takayama, Lin-liu and Maki (1980) and by Campbell and Bishop (1982), that in the continuum limit, and in an approximation that ignores the dynamics of the lattice vibrations, the insulator-metal transition in polyacetylene can be described by the $N = 2$ Gross-Neveu model, i.e. by the Lagrangian density

$$\mathcal{L} = \bar{\psi} i \not{\partial} \psi - g \sigma \bar{\psi} \psi - \frac{1}{2} \sigma^2. \quad (1)$$

This is a $1 + 1$ dimensional model in which ψ is a 2-component Dirac spinor with an internal index that runs over two values (hence $N = 2$). It describes the electronic degrees of freedom of $(CH)_x$, while the auxiliary field $\sigma(x)$ represents the lattice distortion. It is interesting to note, however, that the spin degrees of freedom of the electron are described by the internal index of ψ , while the spinor index of ψ takes account of the right-moving and left-moving electrons

near the Fermi surface. It is also remarkable that polyacetylene can be described, albeit approximately, by a relativistic model. Of course the limiting velocity in the Lorentz group is not the speed of light but rather the Fermi velocity v_F .

Our original motivation in this work was to understand an observed phase transition in polyacetylene, as a function of the concentration of dopants. At a critical concentration of .06 dopants per carbon atom, the data are consistent with a first-order phase transition to a metallic state. We attempt to describe this by computing the effective potential of the GN -model in the presence of a chemical potential h . The role of h is to account for the extra density of electrons that is supplied to the system by the dopants. It is introduced by adding a term $h\psi^\dagger\psi$ to the Hamiltonian of the system.

The behavior of the GN model at finite temperature and density has received considerable attention over the years. We note in particular the work of Wolff (1985), of Karsch, Kogut and Wyld (1987), of Osipov and Fedyanin (1987) and of Klimenko (1988). In our case, we are interested in the effect of the chemical potential (or electron density) with the temperature set to zero. We recall that, in leading order in the $1/N$ expansion, the zero-chemical-potential GN model exhibits spontaneous breaking of discrete chiral symmetry (as well as other interesting phenomena like asymptotic freedom and dimensional transmutation). This corresponds nicely to the degenerate ground state of $trans - (CH)_x$.

As the chemical potential is increased from zero, one finds that at a certain value, $h = m/\sqrt{2}$, where m is the (dynamically-generated) mass of the fermion, the system undergoes a first order phase transition in which the symmetry is restored. The dynamical mass goes to zero above the transition point.

Remarkably enough, the critical value of h that is found above corresponds to a dopant concentration of .06. Furthermore, the transition from the soliton-dominated broken phase to the unbroken phase in which the fermions behave like a free gas is consistent with the observed transition in which the electronic properties resemble those of a metal. And the data also suggest that the transition is first-order (Tsukamoto 1992; Chen, et al. 1985; Moraes, et al. 1985).

The puzzling aspect of all this is why the agreement between theory and experiment should be so good. Not only are we using the GN model, which is an approximation to the lattice Hamiltonian of Su, Schrieffer and Heeger (1980), but the results have been obtained in leading order in the $1/N$ expansion, and, as we have already remarked, the correspondence between the GN model and polyacetylene requires $N = 2$. (In fairness, one should note that $N = 2$ refers to 2 Dirac fermions; in the literature one often calls this the $N = 4$ model, because there are 4 Majorana fermions. Thus a simple change of notation would appear to improve the validity of the approximation significantly.)

Ideally, one would like to solve the thermodynamics of the $N = 2$ GN model exactly. This is not totally out of the question, because the S -matrix, which as we shall see below is the required input for the TBA , is known exactly (Karowski and Thun 1981), and in fact work is in progress to solve the TBA (at zero temperature) for the $N = 2$ GN model numerically (Chodos, Klümper and Minakata, 1997). However, in the remainder of this note we shall discuss the

problem of extending the analysis to the next-to-leading order in $1/N$. This should at least give us some indication as to whether the corrections might significantly affect the location, or even the existence, of the phase transition we have already found.

The straightforward way to go beyond leading order would be to compute the effective potential for the *GN* model to next-to-leading order in $1/N$, including the corrections due to a non-vanishing chemical potential. The analogous computation at zero chemical potential was performed long ago by Schonfeld (1975) and by Root (1975), and an inspection of their work reveals that it is already at a level of complexity that the labor required to incorporate $h \neq 0$ seems excessive. We choose instead to attack the problem through the use of the *TBA*.

Perhaps the most interesting feature of this investigation is simply the discovery of how to establish the correspondence between the results obtained directly from the effective potential and the information contained in the *TBA*. We shall find that, with the exception of a single dimensionless constant, we can recover all the information about the phase transition from the *TBA*. Furthermore, the unknown constant can be obtained from the effective potential evaluated at zero chemical potential. Once this has been understood and the correspondence has been verified to leading order in $1/N$, going to next order is simply a matter of making use of results already in the literature and performing one integral numerically. It remains an interesting question whether even the missing constant can be extracted from the *TBA*, so that, given the *S*-matrix the *TBA* would provide a self-contained and complete description of the thermodynamics of the *GN* system.

The thermodynamic Bethe Ansatz, in a non-relativistic setting, appears in the classic paper by Yang and Yang (1969). The zero-temperature version can be found in the earlier work of Lieb and Liniger (1963). More recent work, including the extension to relativistic field theory, can be found in the papers of Thacker (1981), Zamolodchikov (1990), Klassen and Melzer (1991), and Forgacs, et al. (1991a; 1991b).

At zero temperature, the essence of the *TBA* is a linear integral equation for the dressed single-particle excitation energy $\epsilon(\theta)$. Here θ is the rapidity of the particle: $E = m \cosh \theta$, $p = m \sinh \theta$. The equation reads:

$$\epsilon = h - m \cosh \theta + \int_{-B}^B d\theta' K(\theta - \theta') \epsilon(\theta') \quad (2)$$

where the kernel K is the logarithmic derivative of the *S*-matrix:

$$K(\theta) = \frac{1}{2\pi i} \frac{d}{d\theta} \ln S(\theta). \quad (3)$$

[The *TBA* applies to theories in $1+1$ dimension, such as the *GN* model, where there is only two-body scattering and the *S*-matrix is therefore only a phase factor depending on the relative rapidities of the two particles.] The parameter

B is determined by the condition $\epsilon(\pm B) = 0$ (one is implicitly assuming here first, that $\epsilon(-\theta) = \epsilon(\theta)$, and second, that ϵ is positive for $-B < \theta < B$ and negative for $|\theta| > B$).

Once ϵ has been obtained from the solution to this equation, one can compute the free energy density of the system as (Forgacs, et al. 1991a; 1991b)

$$f(h) - f(0) = \frac{-m}{2\pi} \int_{-B}^B d\theta \epsilon(\theta) \cosh \theta. \quad (4)$$

The constant $f(0)$, on dimensional grounds, must have the form $f(0) = -bm^2$, where b is a dimensionless constant. Our notation anticipates the fact that b will turn out to be positive.

One notes that in the GN model, the expansion of $K(\theta)$ begins in order $1/N$, and therefore to leading order eqn. (2) is extremely simple:

$$\epsilon(\theta) = h - m \cosh \theta \quad (5)$$

with B determined by $\cosh B = h/m$. We see that this is only possible (for real B) if $h \geq m$, and so we have

$$f(h) - f(0) = \frac{-m^2}{2\pi} \theta(h - m) \left[\frac{1}{2} \sinh 2B - B \right]. \quad (6)$$

As was shown in (Chodos and Minakata 1997), one finds that the free energy given above can be interpreted as the value of the effective potential $V(\sigma)$ (properly normalized) at the point $\sigma = \sigma_0$ corresponding to the broken vacuum; the computation of the effective potential is, however, considerably more involved than the manipulations described above for the TBA , so the TBA does indeed permit a much more efficient evaluation of the free energy.

There is, however, an essential point which demands resolution. Where is the evidence for a phase transition? From the effective potential, one learns that there is a first order transition at $h = m/\sqrt{2}$, but the free energy obtained from the TBA is absolutely flat at $h = m/\sqrt{2}$, having non-trivial functional dependence on h only for $h \geq m$. For $h > m/\sqrt{2}$, the expression for the free energy obtained from the effective potential that agrees with the TBA is not actually the value from the true minimum. Rather, as stated above, it is from the point representing the broken vacuum, which ceases to be the global minimum for $h > m/\sqrt{2}$.

To resolve this difficulty, one must recognize that there are really two phases involved: the massive phase characteristic of spontaneously broken chiral symmetry, and described by eqn. (6), and a massless phase corresponding to the restoration of this symmetry. One can obtain the free energy for this phase simply by taking the limit as $m \rightarrow 0$ (with h fixed) of eqn. (6), recognizing that $f(0)$ vanishes in this limit. The result is

$$f_0(h) = \frac{-h^2}{2\pi} . \quad (7)$$

The system will choose to be in whichever of the two phases has the lower free energy, and if there is a value of h for which $f(h) = f_0(h)$, the system will undergo a phase transition at that point.

In order to make this comparison, we need to know the constant b that appears in the formula

$$f(0) = -bm^2 . \quad (8)$$

If $0 < b < 1/2\pi$, then the phase transition will occur at $h/m = \sqrt{2\pi b}$.

According to our present understanding, the *TBA* itself does not determine b . However, within the effective potential formalism, $f(0)$ is the difference $V_0(\sigma_0) - V_0(0)$, where $V_0(\sigma)$ is the effective potential computed at zero chemical potential (up to a normalization factor of $1/N$, this is just the effective potential computed originally by Gross and Neveu) and σ_0 is the value of V_0 at its minimum. By consulting Gross and Neveu's original work (1974), one obtains

$$b = 1/4\pi \quad (9)$$

and hence at the transition $h = m/\sqrt{2}$, reproducing the result from the effective potential.

It is now straightforward to extend this reasoning to next order in $1/N$. The steps are the following:

(a) One makes use of the results of Schonfeld and Root (in particular, in (Chodos and Minakata 1997) we employed an integral formula due to Schonfeld (1975)) to obtain the correction, at zero chemical potential, to $V_0(\sigma)$ of Gross and Neveu. One finds thereby that $b \rightarrow b + \Delta b$, with $\Delta b = (-\frac{1}{4\pi})\frac{2 \cdot 12}{3N}$.

(b) One inserts into the *TBA* the first non-vanishing contribution to K , which occurs at order $1/N$. Following the work of Forgacs, et al. (1991a), we assume that only the S -matrix describing the scattering of fundamental fermions is relevant. [If this is not the case, there will be further, presumably smaller, corrections to this order, but we should still obtain a result that is qualitatively correct.]

(c) One takes the massless limit of the free energy obtained in part (b), giving $f_0(h) = \frac{-1}{2\pi}(1 + \delta)h^2$, with $\delta = (\frac{232}{N})$.

One then makes the same comparison between $f(h)$ and $f_0(h)$ that one did in leading order, to see to what extent the phase transition point has been shifted.

The result for the new critical h is

$$h = \frac{m}{\sqrt{2}} [1 + (\frac{-47}{N})] \quad (10)$$

which for $N = 2$ amounts to about a 20% correction. Since, in the massless phase, the dopant concentration is directly proportional to the chemical potential (see Chodos and Minakata, 1994), this implies that the critical concentration of dopants is about 20% lower, not quite as good as the leading order result, but still comfortably compatible with experiment.

Let us conclude with a few remarks concerning a class of models for which the TBA is exactly solvable. These models *a priori* have nothing to do with the GN model that is our principal concern in this paper, but being exactly solvable they can provide some insight concerning the behavior and mathematical properties of eqn. (2).

The simplest such model has a kernel given by

$$K(\theta) = \lambda \cosh \theta . \quad (11)$$

It is not hard to show that the corresponding S -matrix is $S(p_1, p_2) = e^{i\Phi}$, $\Phi = \frac{2\pi\lambda}{m^2} \epsilon_{\mu\nu} p_1^\mu p_2^\nu$ where $\theta = \theta_1 - \theta_2$, and p_1 and p_2 are the 4-momenta of the scattered particles. This S satisfies the appropriate restrictions imposed by analyticity, unitarity and crossing, but it is not polynomially bounded, and hence it is not clear what kind of underlying degrees of freedom are being described.

In any case, solving the TBA equation one finds

$$\epsilon(\theta) = h - \tilde{m} \cosh \theta \quad (12)$$

where

$$\tilde{m} = \frac{m}{1 + \lambda(\frac{1}{2} \sinh 2B - B)} \quad (13)$$

with $h = \tilde{m} \cosh B$. The free energy becomes

$$f(h) - f(0) = -\theta(h - \tilde{m}) \frac{m^2}{2\pi} \frac{1}{\lambda + [\frac{1}{2} \sinh 2B - B]^{-1}} \quad (14)$$

One can see for $\lambda > 0$ that h is bounded above, and in fact $h \rightarrow 0$ as $B \rightarrow \infty$. For $\lambda < 0$, h can take on all values, in particular $h \rightarrow \infty$ when $B \rightarrow B_c$ given by $1 + \lambda(\frac{1}{2} \sinh 2B_c - B_c) = 0$, but one finds that $\lim_{m \rightarrow 0} f(h) = 0$, so there is no "asymptotically free" behavior in which the free energy has the form $f(h) \rightarrow -\kappa h^2$ for sufficiently large h .

If we study the next simplest model,

$$K(\theta) = \lambda \cosh 3\theta \quad (15)$$

[the case $K = \lambda \cosh 2\theta$ is excluded by crossing symmetry] we again find that this is represented by a non-polynomially bounded S -matrix, and that there is

a marked difference in behavior between positive and negative λ . The solution for ϵ takes the form

$$\epsilon(\theta) = h + \epsilon_1 \cosh \theta + \epsilon_3 \cosh 3\theta . \quad (16)$$

The coefficient ϵ_1 is negative, but for $\lambda > 0$, ϵ_3 is positive. This means that the condition $\epsilon(B) = 0$ is not sufficient to guarantee a solution, because there exists a $B' > B$ such that $\epsilon(\theta) > 0$ for $|\theta| > B'$. We conclude that no solution exists for $\lambda > 0$. For $\lambda < 0$, solutions do exist that are qualitatively similar to the $\lambda < 0$ solutions of the previous example; i.e., they do not exhibit the asymptotic freedom that would allow for the existence of a massless phase such as is found in the *GN* model.

Some of the questions regarding these models are: (a) is it possible to discover what the underlying degrees of freedom are? (b) can one find an example that is more "realistic" (in the sense that it shares the important features of the *GN* model)? (c) can one use these models as a laboratory for understanding how to derive the constant $f(0)$ directly from the *TBA*?

Finally, we conjecture that it may be possible to expand a physically interesting (i.e. one derived from a polynomially bounded *S*-matrix) kernel $K(\theta)$ in a series

$$K(\theta) = \sum_{n=0}^{\infty} C_n \cosh(2n+1)\theta . \quad (17)$$

This would reduce the original *TBA* equation to a matrix equation for the coefficients ϵ_n in the expansion

$$\epsilon(\theta) = h + \sum_{n=0}^{\infty} \epsilon_n \cosh(2n+1)\theta \quad (18)$$

which in turn might bring the problem to a more tractable mathematical form.

Our overall assessment of the status of this work is as follows: we have shown that the Gross-Neveu model appears to give a remarkably good description of the finite-density phase transition observed in polyacetylene, and that the result is stable against higher-order $1/N$ corrections. Numerical work is in progress to solve the *TBA* integral equation exactly for the case of interest. Deeper questions remain, such as whether the *TBA* can provide a complete account of the thermodynamics of the *GN* model, and whether models can be found which permit the exact solution of the *TBA* equation while at the same time making unambiguous physical sense.

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